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A matrix method for computing Szeged and vertex PI indices of join and composition of graphs

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Abstract

The Szeged index extends the Wiener index for cyclic graphs by counting the number of vertices on both sides of each edge and sum these counts. Klavzar et al. [S. Klavzar, A. Rajapakse, I. Gutman, The Szeged and the Wiener index of graphs, Appl. Math. Lett. 9 (5) (1996) 45–49] provided an exact formula for computing Szeged index of product of graphs. In this paper, we apply a matrix method to obtain exact formulae for computing the Szeged index of join and composition of graphs. The join and composition of the vertex PI index of graphs are also computed.

Keywords: Szeged index; Vertex PI index; Graph join; Graph composition

1. Introduction

Throughout this paper graph means finite graph. A topological index of a graph G is a numerical invariant of G. The Wiener index is the first topological index defined by chemist Wiener [24]. Mathematical properties and chemical applications of the Wiener index have been intensively studied in the last 30 years [1–3,6,20,21].

The Szeged index is another topological index introduced by Ivan Gutman at the Attila Jozsef University in Szeged, and so it was called the Szeged index, denoted by Sz, [8]. It is useful to mention here that Gutman in his 1994 paper proposed the existence of the cyclic index and abbreviated it by W^*. In that paper he has not given any name to this index. It was in [13] the index named

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Szeged index and abbreviated as Sz. For more information about Szeged index and its applications in chemistry and biology we encourage the reader to consult [4,5,7–9,11,13,14,16–19,22,25–27].

To define the Szeged index of a connected graph G, we assume that $e = uv$ is an edge connecting the vertices u and v. Suppose $n_u(e|G)$ is the number of vertices of G lying closer to u and $n_v(e|G)$ is the number of vertices of G lying closer to v. Vertices equidistant from u and v are not taken into account. Suppose $e = xy$ is an edge of G and define $\mathrm{Sz}(e) = n_x(e|G)n_y(e|G)$. Then the Szeged index of the graph G is defined as $\mathrm{Sz}(G) = \sum_{e\in E(G)} \mathrm{Sz}(e) = \sum_{e=uv\in E(G)} n_u(e|G)n_v(e|G)$.

We now define the vertex PI index of a graph G, $\mathrm{PI}_v(G)$, as the sum of $[n_u(e|G) + n_v(e|G)]$ over all edges of G, where $n_u(e|G)$ and $n_v(e|G)$ are defined as above. The presented authors in [15] proved that for a graph G, $\mathrm{PI}_v(G) \leqslant |E(G)||V(G)|$ with equality if and only if G is bipartite. They also computed an exact formula for the vertex PI index of product graphs.

Throughout this paper our notation is standard and taken mainly from [10,12,23]. For a $n \times n$ matrix$A = [a_{ij}]$, A^{t} denotes the transpose of matrix A, $A_d = [b_i]$ is an $1 \times n$ matrix defined by $b_i = a_{ii}$ and $A_d^{\mathrm{t}} = (A_d)^{\mathrm{t}}$.

2. Main results and discussion

In the literature, there is a paper by Khadikar et al. [13] described various applications of Szeged index for modeling physicochemical properties as well as physiological activities of organic compounds acting as drugs possess pharmacological activity. The authors of this paper reviewed 175 papers published on the subject of Szeged index. This shows that the subject of Szeged index is more and more growing in science.

The join $G = G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2, [10]. If $G = \underbrace{H + \cdots + H}_{n\ \text{times}}$ then we denote G by nH. The composition $G = G_1[G_2]$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph with vertex set $V_1 \times V_2$ and $u = (u_1, v_1)$ is adjacent with $v = (u_2, v_2)$ whenever (u_1 is adjacent with u_2) or ($u_1 = u_2$ and v_1 is adjacent with v_2), see [12, p. 22]. In [21], Sagan et al. computed some exact formulae for the Wiener polynomial of various graph operations containing join and composition. In [16], Klavzar et al. independent from Sagan and his co-authors computed the Wiener index of product of graphs. They also calculated the Szeged index of product of graphs, as well as the Szeged index of join of k-regular triangle-free graphs. One of the aims of this section is generalizing this result.

Let G and H be graphs with $V_1 = V(G)$, $V_2 = V(H)$, $E_1 = E(G)$, $E_2 = E(H)$, $V = V(G + H)$ and $E = E(G + H)$. Then one can see that $E(G + H) = E_1 \cup E_2 \cup \{v_1v_2 | v_1 \in V_1; v_2 \in V_2\}$. It is easy to see that for every vertices $u, v \in G + H$, $d(u, v) = 1, 2$. Moreover, $d(u, v) = 1$ if and only if one of the following holds:

(a) $u, v \in V_1$ and $d_G(u, v) = 1$,
(b) $u, v \in V_2$ and $d_H(u, v) = 1$,
(c) $u \in V(G)$ and $v \in V(H)$.

Let G be a graph and $A(G)$, $M(G)$ denote the adjacency and incidence matrices of G, respectively. The $M(G)$ and $A(G)$ are said to be consistent if they obtained according to a fixed ordering of $V(G)$. In what follows, $N_1 = \{1, 2, \ldots, n\}$ and $t(e)$, $e \in E(G)$, denote the number of triangles containing e. Moreover, $t(G)$ denotes the number of triangles of the graph G and $J_{m\times n} = [x_{ij}]$ is defined as $x_{ij} = 1$ for all $1 \leqslant i \leqslant m$ and $1 \leqslant j \leqslant n$.

Theorem 1. *Let G be a graph, $A(G)$ be consistent with M(G), $B = M(G)^{\mathrm{t}}A(G)$, $D = BB^{\mathrm{t}}$ and $F = A(G)J_{n\times 1}$, where $n = |V(G)|$. Then*

$$\sum_{uv=e\in E(G)} (\deg(u) - t(e))(\deg(v) - t(e)) = 1/4(5J_{1\times n}B^{\mathrm{t}}BJ_{n\times 1} - 4D_dBJ_{n\times 1} + D_dD_d^{\mathrm{t}} - 2(FF^{\mathrm{t}})_dF).$$

Proof. Suppose $\bar{e}$ is an arbitrary row of $M(G)^{\mathrm{t}}$ corresponding to the edge $e = ab \in E(G)$ and $\bar{v}$ is an arbitrary column of $A(G)$ corresponding to the vertex $v \in V(G)$. Then by consistency of $M(G)$ and $A(G)$,

$$\bar{e}\cdot\bar{v} = \begin{cases} 0 & d(v,a), d(v,b) > 1, \\ 1 & (d(v,a), d(v,b) = 0 \text{ or } 1) \text{ and } (d(v,a) \neq d(v,b)), \\ 2 & d(v,a) = d(v,b) = 1, \end{cases} \tag{1}$$

Therefore, the sum of entries of the row of $M(G)^{\mathrm{t}} \times A(G)$ corresponding to e is $\deg(u) + \deg(v)$. On the other hand, by Eq. (1) the sum of squares of entries in this row is equal to $\deg(u) + \deg(v) + 2t(e)$. So,

$$4\sum_{uv=e\in E(G)} (\deg(u) - t(e))(\deg(v) - t(e)) - \sum_{uv=e\in E(G)} (\deg(u) + \deg(v))^2 + 2\sum_{uv=e\in E(G)} (\deg(u)^2 + \deg(v)^2) = (2J_{1\times n}B^{\mathrm{t}} - (BB^{\mathrm{t}})_d)(2BJ_{n\times 1} - (BB^{\mathrm{t}})_d^{\mathrm{t}}). \tag{2}$$

By above discussion, the ith entry of vectors appeared in the right hand side of Eq. (2) is equal to $\deg(u) + \deg(v) - 2t(e)$, where $\bar{e}$ is the ith row of $M(G)^{\mathrm{t}}$. Also,

$$\sum_{uv=e\in E(G)} (\deg(u) + \deg(v))^2 - 2\sum_{uv=e\in E(G)}(\deg(u)^2 + \deg(v)^2) = J_{1\times n}B^{\mathrm{t}}BJ_{n\times 1} - 2(A(G)J_{n\times n}A(G))_dA(G)J_{n\times 1}.$$

It is clear that, $\sum_{uv=e\in E(G)} (\deg(u) + \deg(v))^2 = J_{1\times n}B^{\mathrm{t}}BJ_{n\times 1}$. On the other hand, one can see that for every $v_i \in V(G)$, $\deg(v_i)^2$ appear $\deg(v_i)$ times in $\sum_{uv=e\in E(G)} (\deg(u)^2 + \deg(v)^2)$. Therefore, $\sum_{uv=e\in E(G)} (\deg(u)^2 + \deg(v)^2) = \sum_{v\in V(G)} \deg(v)^3 = (A(G)J_{n\times n}A(G))_d A(G)J_{n\times 1}$. Thus

$$\begin{aligned} 4\sum_{uv=e\in E(G)} &(\deg(u) - t(e))(\deg(v) - t(e)) \\ &= (2J_{1\times n}B^{\mathrm{t}} - (BB^{\mathrm{t}})_d)(2BJ_{n\times 1} - (BB^{\mathrm{t}})_d^{\mathrm{t}}) + J_{1\times n}B^{\mathrm{t}}BJ_{n\times 1} - 2(A(G)J_{n\times n}A(G))_dA(G)J_{n\times 1} \\ &= 4J_{1\times n}B^{\mathrm{t}}BJ_{n\times 1} - 2J_{1\times n}B^{\mathrm{t}}(BB^{\mathrm{t}})_d^{\mathrm{t}} - 2(BB^{\mathrm{t}})_dBJ_{n\times 1} + (BB^{\mathrm{t}})_d(BB^{\mathrm{t}})_d^{\mathrm{t}} \\ &\quad + J_{1\times n}B^{\mathrm{t}}BJ_{n\times 1} - 2(A(G)J_{n\times n}A(G))_dA(G)J_{n\times 1}. \end{aligned}$$

Now by our assumption and that $J_{1\times n}B^{\mathrm{t}}(BB^{\mathrm{t}})_d = (BB^{\mathrm{t}})_d^{\mathrm{t}}BJ_{n\times 1}$, we have

$$4\sum_{uv=e\in E(G)} (\deg(u) - t(e))(\deg(v) - t(e)) = 5J_{1\times n}B^{\mathrm{t}}BJ_{n\times 1} - 4D_dBJ_{n\times 1} + D_dD_d^{\mathrm{t}} - 2(FF^{\mathrm{t}})_dF,$$

which completes our proof. □

Theorem 2. *Let $G_1, \ldots, G_n$ be graphs and $G = G_1 + G_2 + \cdots + G_n$. Then we have*

$$\mathrm{Sz}(G) = 1/4\sum_{i=1}^{n}[5J_{1\times n}B_i^{\mathrm{t}}B_iJ_{n\times 1} - 4(D_i)_dB_iJ_{n\times 1} + (D_i)_d(D_i)_d^{\mathrm{t}} - 2(F_iF_i^{\mathrm{t}})_dF_i] + \frac{1}{2}\left(\sum_{i=1}^{n}[|V_i|^2 - 2|E_i|]\right)^2 - \frac{1}{2}\sum_{i=1}^{n}[|V_i|^2 - 2|E_i|]^2,$$

where $V_i = V(G_i)$, $E_i = E(G_i)$, $B_i = M(G_i)^{\mathrm{t}}A(G_i)$, $D_i = B_i(B_i)^{\mathrm{t}}$ *and* $F_i = A(G_i)J_{|V_i|\times 1}$, $1 \leqslant i \leqslant n$.

Proof. By definition of the join of graphs, one can see that $V(G) = \bigcup_{i=1}^{n} V_i$ and $E(G)=\bigcup_{i=1}^{n} E_i \bigcup \left(\bigcup_{\{i,j\}\subseteq N_1} \{v_iv_j|v_i \in V_i, v_j \in V_j\}\right)$. Obviously, $G_1 + G_2 \cong G_2 + G_1$. Consider an edge $e = uv \in E(G)$, $u \in V_i$, $v \in V_j$ and $i \neq j$. Then $d(u, w) = 1$, $w \in V_k, k \neq i$. If $wu \in E_i$, $w \in V_i$ then $d(u, w) = 1$. Also, the number of such vertices $w \in V_i$ is equal to $\deg_{G_i}(u)$ and u has distance 2 with other vertices of V_i except from u. The similar property is valid for the vertex v and so $n_u(uv|G) = |\{v_j \in V_j|d(v, v_j) = 2\}| + |\{v_i \in V_i|d(u, v_i) < 1\}| = (|V_j| - \deg_{G_j}(v) - 1) + 1$. Therefore,

$$\begin{aligned}
&\textstyle\sum_{\{i,j\}\subseteq N_1} \sum_{u\in V_i} \sum_{v\in V_j}(|V_i| - \deg_{G_i}(u))(|Vj| - \deg_{G_j}(v))\\
&\quad = \textstyle\sum_{uv=e\in E(G)-\bigcup E_i} n_u(e|G)n_v(e|G)\\
&\quad = \tfrac{1}{2}\left(\sum_{i=1}^{n}[|V_i|^2 - 2|E_i|]\right)^2 - \tfrac{1}{2}\sum_{i=1}^{n}[|V_i|^2 - 2|E_i|]^2.
\end{aligned}$$

Consider $uv \in E_k$. By definition of join, if $b \notin V_k$ then $d(v, b) = d(u, b) = 1$; if $u \in V_k$ and $d_{G_k}(u, x) = 1$ then $d(u, x) = 1$ and for other vertices as $x \in V_k - u$, $d(u, x) = 2$. Since $n_u(e|G) = |\{w \in V(G)|d(u, w) < d(v, w)\}| = |\{w|d_{G_k}(u, w) = 1 \text{ and } d(v, w) = 2\}| + |\{w|d_{G_k}(u, w) = 0 \text{ and } d_{G_k}(v, w) = 1\}| = |\{w|d_{G_k}(u, w) = 1\}| - |\{w|d_{G_k}(u, w) = 1 \text{ and } d(v, w) = 0\}| - |\{w|d_{G_k}(u, w) = 1 \text{ and } d_{G_k}(v, w) = 1\}| + 1 = \deg_{G_k}(u) - t_{G_k}(uv)$. Thus $\sum_{e=uv\in E_i} n_u(e|G)n_v(e|G) = \sum_{e=uv\in E_i} (\deg_{G_k}(u) - t_{G_k}(e))(\deg_{G_k}(v) - t_{G_k}(e))$. We now apply Theorem 1, the equation $G_1 + G_2 \cong G_2 + G_1$ and the following equations

$$\begin{aligned}
\mathrm{Sz}(G) &= \textstyle\sum_{e\in E(G)-\cup E_i} n_u(e|G)n_v(e|G) + \sum_{e\in\cup E_i} n_u(e|G)n_v(e|G)\\
&= \tfrac{1}{2}\textstyle\sum_{i,j=1,i\neq j}^{n} \sum_{u\in V_i} \sum_{v\in V_j} (|V_i| - deg_{G_i}(u))(|V_j| - deg_{G_j}(v)),\\
&\quad + \textstyle\sum_{i=1}^{n} \sum_{e=uv\in E_i} (\deg_{G_i}(u) - t_{G_i}(e))(\deg_{G_i}(v) - t_{G_i}(e)).
\end{aligned}$$

to complete the proof. □

Corollary 1. *With notations of Theorem* 2, *we have*

$$\mathrm{Sz}(G) = \frac{1}{2}\sum_{i=1}^{n}\mathrm{Sz}(G_i + G_i) + \frac{1}{2}\left(\sum_{i=1}^{n}(|V_i|^2 - 2|E_i|)\right)^2 - \sum_{i=1}^{n}(|V_i|^2 - 2|E_i|)^2.$$

Moreover, for a graph H, $\mathrm{Sz}(nH) = \frac{n}{2}\mathrm{Sz}(2H) + \left(\binom{n}{2} - \frac{n}{2}\right)(|V(H)|^2 - 2|E(H)|)^2$.

Proof. Apply Theorems 1 and 2. □

In the following examples, we apply Theorem 2 to compute the Szeged index of a complete graph K_n and r-partite graph $K_{n_1,n_2,\ldots,n_r}$.

Example 1. In this example we compute the Szeged index of a complete graph K_n. Since $K_n = nK_1$, by the previous Corollary, $\mathrm{Sz}(K_n) = \frac{n}{2}\mathrm{Sz}(K_2) + \left(\binom{n}{2} - \frac{n}{2}\right) = \binom{n}{2}$.

Example 2. In this example, we compute the Szeged index of an n-partite graph. At first, we notice that the join of n arbitrary graphs, $n > 1$, are connected. On the other hand, the r-partite graph $K_{n_1,n_2,\ldots,n_r}$ is the join of r empty graph $G_1, G_2, \ldots, G_r$ with exactly $n_1, n_2, \ldots, n_r$

vertices, respectively. So $A(G_i)$, $M(G_i)$ are zero matrices and by Theorem 2, $\mathrm{Sz}(K_{n_1,n_2,\ldots,n_r}) = \mathrm{Sz}(G_1 + \cdots + G_n) = 1/2\sum_{i,j=1,i\neq j}^{r} n_i^2 n_j^2$.

Lemma 3. *With notations of Theorem 2, suppose that G_1 and G_2 are triangle free graphs. Then* $\mathrm{Sz}(G_1 + G_2) = (|V_1|^2 - 2|E_1|)(|V_2|^2 - 2|E_2|) + (1/2)(J_{1\times n}B_1^{\mathrm{t}}B_1J_{n\times 1} + (F_1F_1^{\mathrm{t}})_dF_1 + J_{1\times n}B_2^{\mathrm{t}}B_2J_{n\times 1} + (F_2F_2^{\mathrm{t}})_dF_2)$.

Proof. Apply Theorem 2. □

Corollary 2. *Suppose that $G_1, \ldots, G_n$ are triangle free graphs k_j regular graphs, respectively. Then* $\mathrm{Sz}(G_1 + \cdots + G_n) = (1/2)[\sum_i |V_i|(|V_i| - k_i)]^2 - (1/2)\sum_i |V_i|^4(1 - 2k_i/|V_i| + k_i^2/|V_i|^2 - k_i^3/|V_i|^3)$.

In Corollary 1.35 of [12], Imrich and Klavzar proved a result relating to the distance between two vertices of Cartesian product of graphs. In the following simple lemma, we extend this result to graphs composition.

Lemma 4. *Let G_1 be connected, $|V_1| > 1$ and $G = G_1[G_2]$. For every vertices $(u_1, v_1), (u_2, v_2) \in V(G)$ we have*

$$d_G((u_1,v_1),(u_2,v_2)) = \begin{cases} d_{G1}(u_1,u_2), & u_1 \neq u_2,\\ 0, & u_1 = u_2 \text{ and } v_1 = v_2,\\ 1, & u_1 = u_2 \text{ and } v_1v_2 \in E_2,\\ 2, & u_1 = u_2 \text{ and } v_1v_2 \notin E_2. \end{cases}$$

Proof. If $u_1u_2 \in E_1$ then for every vertex $v_1, v_2 \in V_2$, $d_G((u_1,v_1),(u_2,v_2)) = 1 = d_{G_1}(u_1,u_2)$ and if $u_1u_2 \notin E_1$ then by definition, $(u_1,v_1)(u_2,v_2) \notin E(G)$ and so $d_G((u_1,v_1),(u_2,v_2)) = d_{G_1}(u_1,u_2)$. Other cases that $u_1 = u_2$ are immediate consequence of definition. □

Theorem 3. *Let G_1 be connected graph. Then* $\mathrm{Sz}(G) = \mathrm{Sz}(G_1[G_2]) = |V_2|^4\mathrm{Sz}(G_1) - 2|E_2||V_2|^2\mathrm{PI}_v(G_1) + (|V_1|/2)\mathrm{Sz}(2G_2) + 4|E_1||E_2|^2 - (|V_1|/2)(|V_2|^2 - 2|E_2|)^2$.

Proof. Suppose $A_u = \{(u,v)|v \in V_2\}$, $B_u = \{(u,v_1)(u,v_2)|v_1v_2 \in E_2\}$ and $T(u_1,u_2) = \{(x,y)(a,b)|((x,y),(a,b)) \in A_{u_1} \times A_{u_2}\}$. Then $E(G) = (\cup_{u_1u_2\in E_1} T(u_1,u_2)) \cup (\cup_{v\in V_1} B_v)$. We first prove two results which are crucial in our proof.

Claim 1. $\sum_{uv\in\cup_{u_1u_2\in E_1}T(u_1,u_2)} \mathrm{Sz}(uv) = |V_2|^4\mathrm{Sz}(G_1) - 2|E_2|(|V_2|^2\mathrm{PI}_v(G_1) - 2|E_1||E_2|)$.

Suppose $e = (u_1,v_1)(u_2,v_2) \in T(u_1,u_2)$, where $u_1u_2 \in E_1$. Then

$$\begin{aligned} n_{(u_1,v_1)}(e|G) &= |\{(w,t)|d_G((w,t),(u_1,v_1)) < d_G((w,t),(u_2,v_2))\}|\\ &= |\{(w,t)|d_G((w,t),(u_1,v_1)) < d_G((w,t),(u_2,v_2)) \text{ and } (w,t) \notin A_{u_1} \cup A_{u_2}\}|\\ &\quad + |\{(w,t)|d_G((w,t),(u_1,v_1)) < d_G((w,t),(u_2,v_2)) \text{ and } (w,t) \in A_{u_1}\}|\\ &\quad + |\{(w,t)|d_G((w,t),(u_1,v_1)) < d_G((w,t),(u_2,v_2)) \text{ and } (w,t) \in A_{u_2}\}|. \end{aligned}$$

By Lemma 4, $|\{(w,t)|d_G((w,t),(u_1,v_1)) < d_G((w,t),(u_2,v_2)) \text{ and } (w,t) \notin A_{u_1} \cup A_{u_2}, t \in V_2\}| = |V_2|.|\{w|d_{G_1}(w,u_1) < d_{G_1}(w,u_2), w \neq u_1,u_2\}| = |V_2|(n_{u_1}(u_1u_2|G_1) - 1)$, $|\{(w,t)|d_G((w,t),(u_1,v_1)) < d_G((w,t),(u_2,v_2)) \text{ and } (w,t) \in A_{u_1}\}| = |\{(u_1,v_1)\}| = 1$, and $|\{(w,t)|d_G((w,t),(u_1,v_1)) < d_G((w,t),(u_2,v_2)) \text{ and } (w,t) \in A_{u_2}\}| = |A_{u_2}| - |\{(w,t)|d_G((w,t),$

$(u_2, v_2)) = 0, 1\}| = |V_2| - \deg_{G_1}(u_1) - 1$. So, $n_{(u_1,v_1)}(e|G) = |V_2|n_{u_1}(u_1u_2|G_1) - \deg_{G_2}(v_2)$ and by similar argument $n_{(u_2,v_2)}(e|G) = |V_2|n_{u_1}(u_1u_2|G_1) - \deg_{G_2}(v_1)$. Therefore,

$$\begin{aligned}&\textstyle\sum_{e\in T(u_1,u_2)} n_{(u_1,v_i)}(e|G)n_{(u_2,v_j)}(e|G)\\ &\quad= \textstyle\sum_{v_j\in V_2}\sum_{v_i\in V_2}[n_{u_1}(u_1u_2|G_1)|V_2| - \deg_{G_2}(v_i)][n_{u_2}(u_1u_2|G_1)|V_2| - \deg_{G_2}(v_j)]\\ &\quad= [n_{u_1}(u_1u_2|G_1)|V_2|^2 - 2|E_2|][n_{u_2}(u_1u_2|G_1)|V_2|^2 - 2|E_2|].\end{aligned}$$

Since the sets $T(u, v)$, $uv \in E_1$, are disjoint, one can see that

$$\begin{aligned}&\textstyle\sum_{uv\in\cup_{u_1u_2\in E_1}T(u_1,u_2)} \mathrm{Sz}(uv)\\ &\quad= \textstyle\sum_{uv\in E_1}[|V_2|^4 n_u(e|G_1)n_v(e|G_2) + 4|E_2|^2 - 2|E_2||V_2|^2(n_u(e|G_1) + n_v(e|G_2))]\\ &\quad= |V_2|^4\mathrm{Sz}(G_1) - 2|E_2|(|V_2|^2\mathrm{PI}_v(G_1) - 2|E_1||E_2|).\end{aligned}$$

Claim 2. By notation of Theorem 1 for the graph G_2, $\sum_{uv\in\bigcup_{m=1}^{|V_1|}B_{u_m}}\mathrm{Sz}(uv) = \frac{|V_1|}{4}(5J_{1\times n}B^{\mathrm{t}}BJ_{n\times1} - 4D_dBJ_{n\times1} - D_dD_d^{\mathrm{t}} - 2(FF^{\mathrm{t}})_dF)$.

Suppose $e=(u, v_1)(u, v_2)\in B_{u_n}$. By Claim 1, for every $v=(u_k, v_k) \in A_{u_k}$, $k \neq n$, $d_G((u_k, v_k), (u, v_1)) = d_G((u_k, v_k), (u, v_2))$. If $d_{G_2}(v_1, v_k) > 2$ and $d_{G_2}(v_2, v_k) > 2$ then $d_G((u, v_1), v) = d_G((u, v_2), v)$. This shows that $n_{(u,v_1)}(e|G) = |\{v \in V_2|d_{G_2}(v_1, v) = 0, 1$ and $d_{G_2}(v_1, v) \neq d_{G_2}(v_2, v)\}| = \deg_{G_2}(v_1) - t_{G_2}(v_1v_2)$. Similarly, $n_{(u,v_2)}(e|G) = \deg_{G_2}(v_2) - t_{G_2}(v_1v_2)$. Since B_u's are disjoint and the above equalities are independent from u_n, $\sum_{uv\in\bigcup_{m=1}^{|V_2|}B_{u_m}}\mathrm{Sz}(uv) = \sum_{uv\in\bigcup_{m=1}^{|V_1|}B_m} n_u(e|G)n_v(e|G) = \sum_{i=1}^{|V_1|}\sum_{e=uv\in E_2}[(\deg_{G_2}(v) - t_{G_2}(e))(\deg_{G_2}(u) - t_{G_2}(e))] = \frac{|V_1|}{4}(5J_{1\times n}B^{\mathrm{t}}BJ_{n\times1} - D_dBJ_{n\times1} - D_dD_d^{\mathrm{t}} - 2(FF^{\mathrm{t}})_dF)$.

By Corollary 1, $\frac{|V_1|}{4}\left(5J_{1\times n}B^{\mathrm{t}}BJ_{n\times1} - D_dBJ_{n\times1} - D_dD_d^{\mathrm{t}} - 2(FF^{\mathrm{t}})_dF\right) = (|V_1|/2)\mathrm{Sz}(2G_2) - (|V_1|/2)(|V_2|^2 - 2|E_2|)^2$. Since $(\bigcup_{uv\in E_1}T(u, v)) \cap (\bigcup_{m=1}^{|V_1|}B_m) = \emptyset$, $\mathrm{Sz}(G_1[G_2]) = \sum_{e\in\bigcup_{uv\in E_1}T(u,v)}\mathrm{Sz}(e) + \sum_{e\in\bigcup_{m=1}^{|V_1|}B_m}\mathrm{Sz}(e)$. Now by Claims 1 and 2 and the first equality of this paragraph, $\mathrm{Sz}(G_1[G_2]) = |V_2|^4\mathrm{Sz}(G_1) - 2|E_2||V_2|^2\mathrm{PI}_v(G_1) + (|V_1|/2)\mathrm{Sz}(2G_2) + 4|E_1||E_2|^2 - (|V_1|/2)(|V_2|^2 - 2|E_2|)^2$. This completes the proof. □

To prove the second main result of this paper, we need to calculate the vertex PI index of join of n graphs, as well as the Szeged index of the composition of two graphs.

Lemma 5. *Let G_i be graphs with adjacency matrix A_i, $1 \leqslant i \leqslant n$, and $G = G_1 + G_2 + \cdots + G_n$. Then*

(1) $\mathrm{PI}_v(G) = (\sum_i |V_i|(\sum_{j\neq i}(|V_j|^2 - 2|E_j|)) + \sum_i((A_i^2)_d(A_i^2)_d^{\mathrm{t}} - \mathrm{tr}(A_i^3))$,
$=(\sum_i |V_i|)(\sum_i(|V_i|^2 - 2|E_i|)) - 2(\sum_i |V_i|(|V_i|^2 - 2|E_i|)) + (1/2)\sum_i \mathrm{PI}_v(2G_i)$,
(2) $\mathrm{PI}_v(nH) = n(n-2)(|V|^3 - 2|E||V|) + (n/2)\mathrm{PI}_v(2H)$,
(3) $\mathrm{PI}_v(G_1[G_2]) = |V_2|^3(\mathrm{PI}v(G_1) - |V_1|) + (|V_1|/2)\mathrm{PI}_v(2G_2) + 2|E_2||V_2|(|V1| - 2|E_2|)$.

Proof. It is well-known fact that $\sum_{v\in V}\deg(v)^2 = \sum_{uv\in E}[\deg(u) + \deg(v)]$ and $\mathrm{tr}(A_i^3) = 6\cdot t_{G_i}(G_i)$. Then the first part of (1) is obtained from these equations and the proof of Theorem 2. To prove (2), it is enough to apply (1), and, (3) is a consequence of the proof of Theorem 3. □

We are now ready to compute the Szeged index of composition of n graphs. To do this, we again introduce some notation: $G_{r,r} = G_r$, $G_{r,k} = G_r[G_{r+1}[\ldots[G_k]\ldots]]$, $r < k$, and, $G_{r,k} = K_1$, for $r > k$. Moreover, $V(G_{r,k}) = V_{r,k}$ and $E(G_{r,k}) = E_{r,k}$.

Theorem 4. *With notation of the last paragraph, we have*

(1) $\mathrm{PI}_v(G_{1,n}) = \sum_{i=2}^{n} |V_{i+1,n}|^3 \left[\left(\frac{\mathrm{PI}_v(2G_i)}{2} - |V_i|^3\right)|V_{1,i-1}| + 2|E_i||V_i|(|V_{1,i-1}| - 2|E_{1,i-1}|)\right] + |V_{2,n}|^3 \mathrm{PI}_v(G_1)$,

(2) $\mathrm{Sz}(G_{1,n}) = |V_{2,n}|^4 \mathrm{Sz}(G_1) + \sum_{i=2}^{n} |V_{i+1,n}|^4 [\frac{|V_{1,i-1}|}{2}(\mathrm{Sz}(2G_i) - (|V_i| - 2|E_i|)^2) + 2|E_i|[2|E_{1,i-1}||E_i| - |V_i|^2 \mathrm{PI}_v(G_{1,i-1})]]$.

Proof. (1) The case of $n = 2$ is the part (3) of Lemma 5. Suppose $n > 2$. Then by the associativity of composition of graphs, $G_{l,k} \cong G_{l,m}[G_{m+1,k}]$, $l \leqslant m \leqslant k$. Now the proof of (1) needs to an inductive argument and some tedious calculations. (2) The case of $n = 2$ proved in Theorem 3. The general case is a consequence of part 1, the associativity of composition of graphs and an inductive argument. □

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